The Largest Fullerene

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The ground state allotrope of bulk carbon, at temperatures below a few thousand Kelvin and pressures below a few GPa, is graphite [1]. At sizes of tens to hundreds of atoms, fullerenes instead stand out as a particularly stable allotrope [2]. This leads to the question of at what size graphitic materials become thermodynamically favorable over closed-cage fullerenes? Or, in other words, what is the largest fullerene? Here, we have used classical molecular dynamics to investigate this by modeling single- and multi-layered structures of graphene and fullerenes. Of the systems we have studied, single-caged fullerenes are the most stable structures for sizes up to about 10^4 atoms. So-called carbon onions [3], multi-layered fullerenes then become the most stable allotrope at sizes above this and only at sizes above 10^{11} atoms do graphite-like structures become the energetically preferred species. I will present a detailed overview of our calculations and findings.

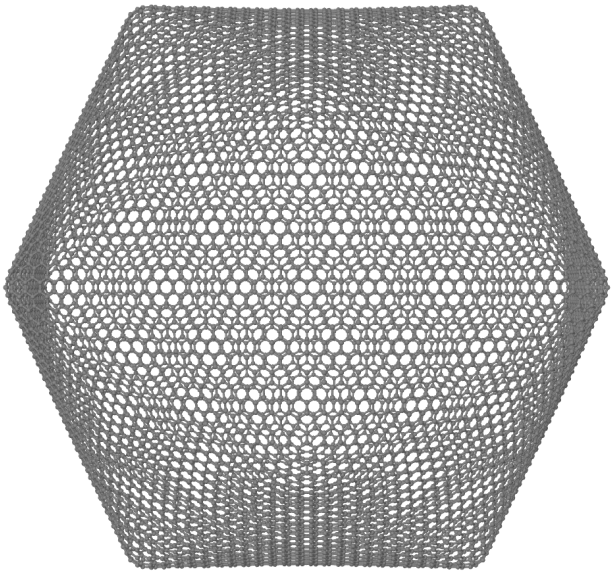

FIG. 1: The optimized structure of the C_{10140} fullerene.

References

[1] F. P. Bundy *et al.*, Carbon **34**, 141–153 (1996).

[2] H. W. Kroto *et al.*, Nature **318**, 162–163 (1985).

[3] H. W. Kroto, Nature **359**, 670–671 (1992).